Nonlinear Model Reduction with Reduced Basis Methods

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Software concept

In order to quickly develop model reduction software for arbitrary evolution systems, we developed a modularized software concept.

The concept's key properties are the following:

1. **minimally intrusive extension:** Enable the rapid exension of a user's favorite PDE solver, so it can be used as a reduced basis scheme.
2. **software decomposition:** High–dimensional computations and low–dimensional computations can be separated for execution on different computer architectures.
3. **reduced basis library**

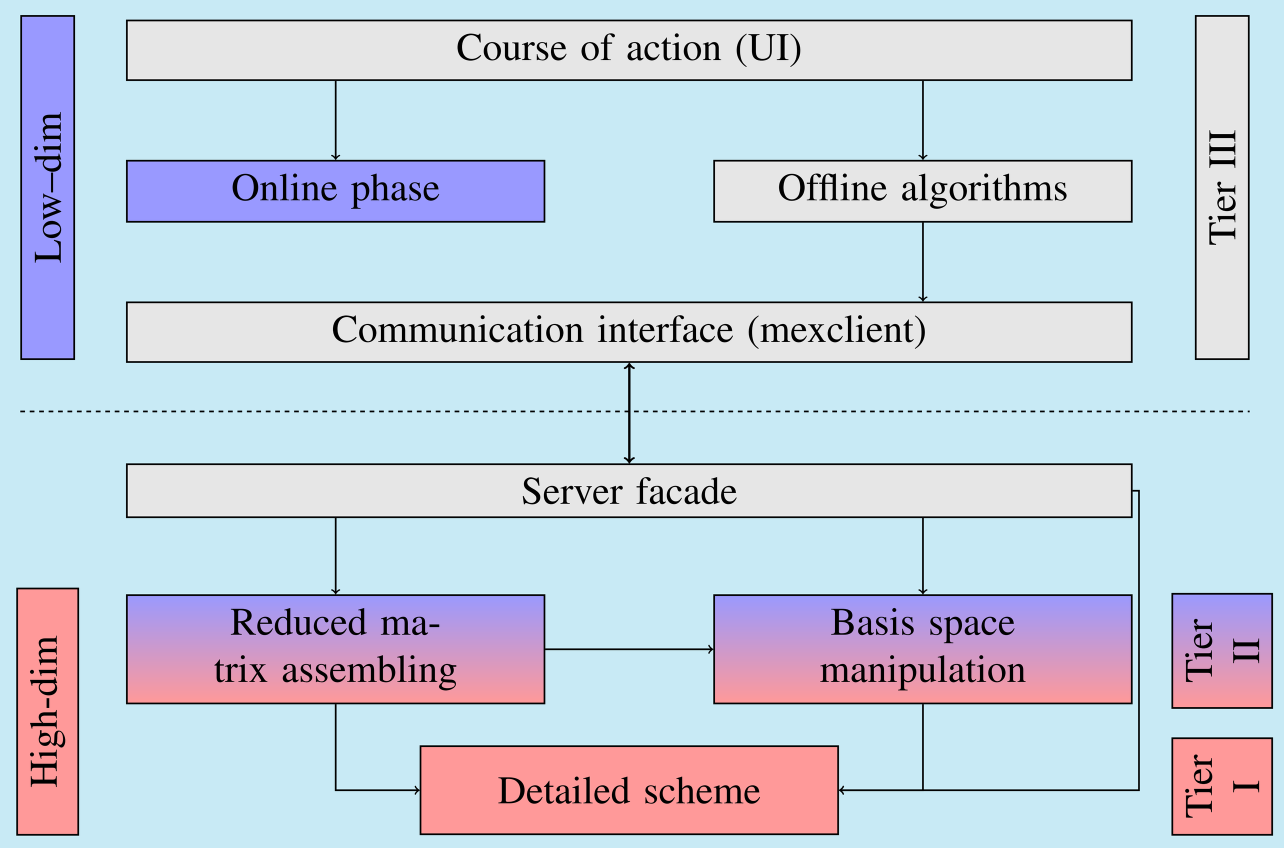


Figure 1: Call graph for main software parts in our abstract software concept. High–dimensional parts can be strictly separated from the low–dimensional ones.

Proof of concept:

- The entire concept was implemented in a *MATLAB* software package called **RBMatlab** (`http://morepas.org/software`)
- The modules from the tiers I and II were also implemented with the *C++* numerics environment **Dune**.
- Dune was developed for efficient development of **HPC applications**.
- The machine learning algorithms for the basis generation during the offline phase, can be easily **parallelized**.

Prospective work at Sandia

- With Kevin Carlberg: Improve **effectivity** of error estimates, incorporate reduced-basis **error estimates as sources of uncertainty** in UQ applications, apply reduced basis methods to **Sandia applications**.
- With Khachik Sargsyan, Gilbert Hendry: Use **uncertainty quantification** methods, in order to predict the performance of HPC software on **exascale** architectures.

Reduced Basis Method

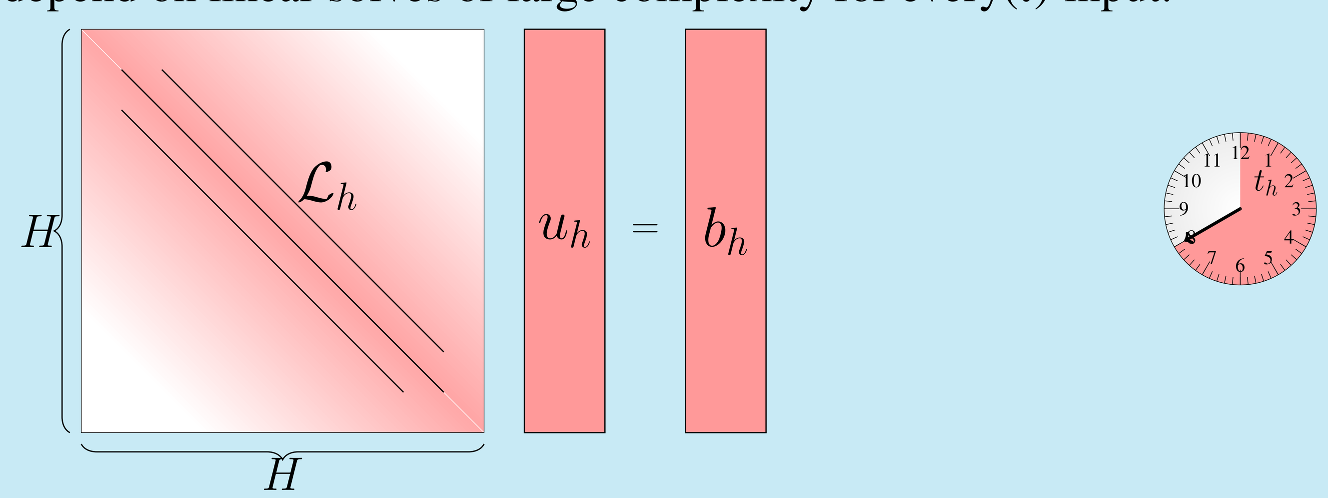
Motivation:
In applications like optimization or uncertainty quantification, numerical simulations must be computed for many different configurations, control variables or inputs. Reduced basis methods can be used to reduce the computational complexity in these cases.

Scenario: Parametrized evolution equations

Inputs: control variable or parameter $\boldsymbol{\mu}$	⟹	**Dynamical system:** usually described by an ordinary differential equation $\partial_t u - \mathcal{L}_h(u;\boldsymbol{\mu}) = 0$	⟹	**Outputs:** trajectory or functional evaluation $s(\boldsymbol{\mu};u)$

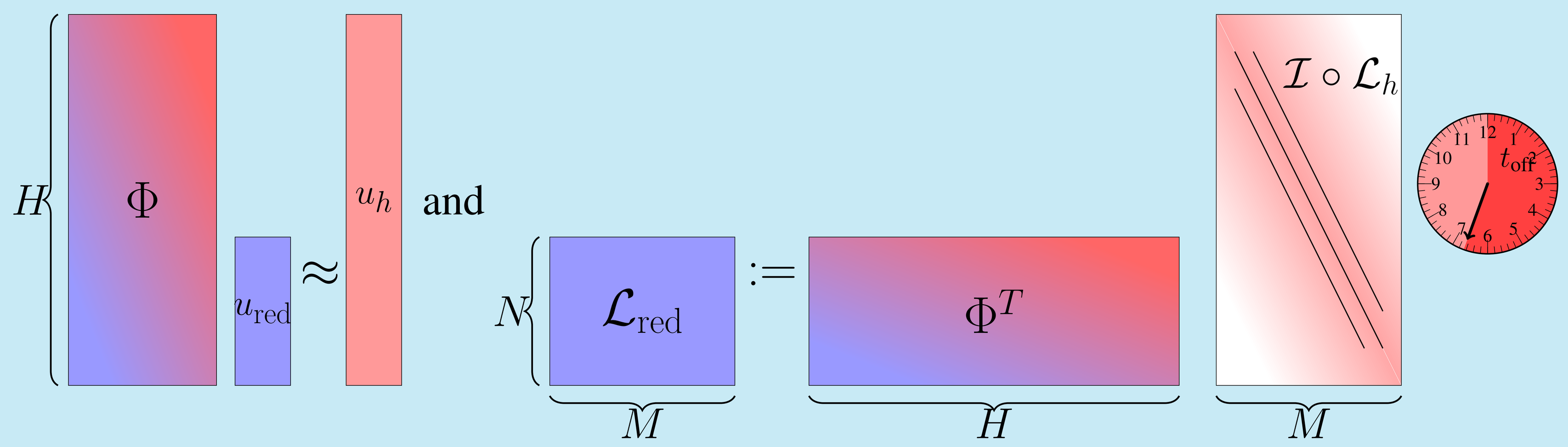
High-dim Simulation

Numerical simulations depend on linear solves of large complexity for every(**!**) input.



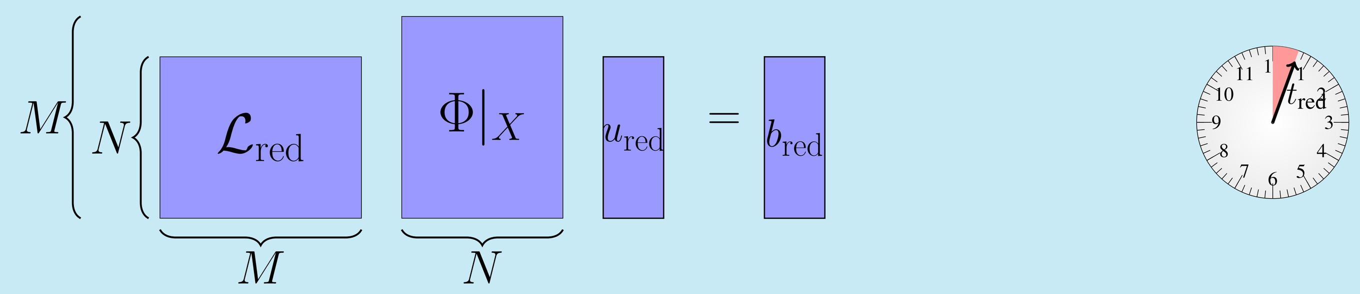
Offline Phase

With machine learning methods (Greedy algorithm, PCA), a **reduced basis** Φ and an **empirical operator interpolation** are derived. This leads to **pre–computable** low–dimensional quantities.



Online Phase

The computational complexity is **massively reduced**, because the linear solves depend only on $N, M \ll H$ for every(**!**) input.



Amortization:
Reduced-basis model reduction pays off if

- the application depends on **many queries**.
- an output must be computed in **real time**.

Error Estimation:
The approximation error can be controlled **efficiently** and **rigorously** with an error bound $\eta(\boldsymbol{\mu})$:

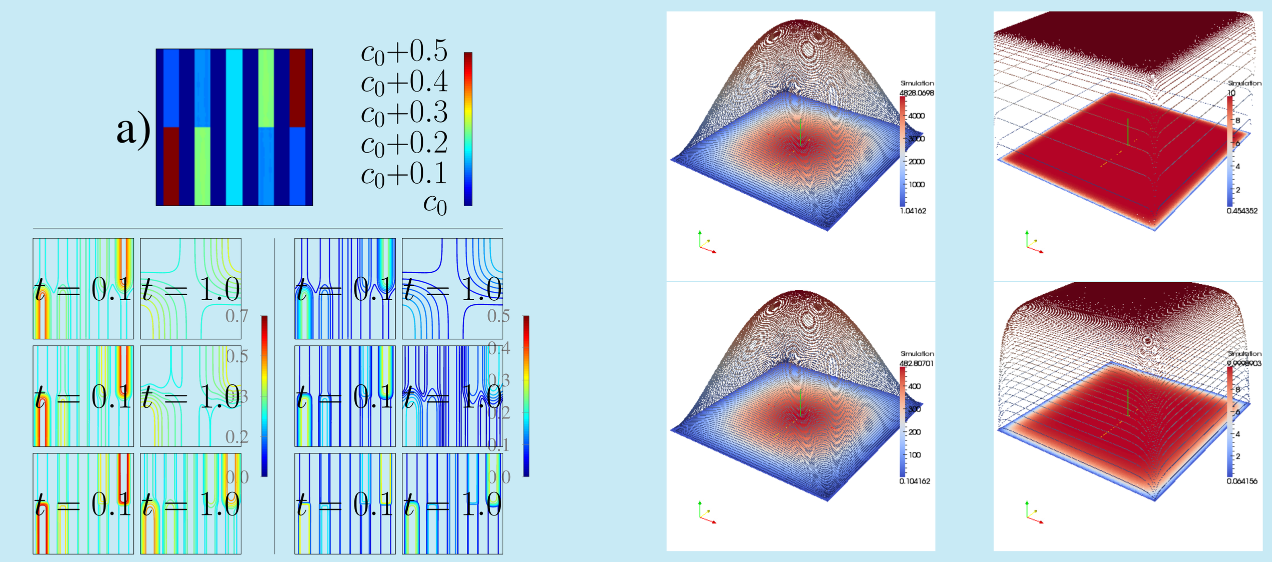
$$\|u_h(\boldsymbol{\mu}) - u_{\mathrm{red}}(\boldsymbol{\mu})\| \leq \eta(\boldsymbol{\mu})$$

Experiments

Results:

- Numerical experiments were evaluated for problems motivated by applications in **computational fluid dynamics**.
- The reduced basis method was applied to **linear** and **non–linear** problems.
- The PDEs were discretized with **finite volume** schemes on a structured mesh.
- The reduced simulations preserve important properties like **conservation**.

Sample snapshots:



Time gain:

- Non–linear problems: approximately **1-2 orders of magnitude**.
- Linear problem: more than **4(!) orders of magnitude**.

non–linear

N	M	ø-run–time[s]	max. error	offline time[h]
$H = 7200$	–	90.01	0.00	0
42	83	4.42	$1.15 \cdot 10^{-3}$	0.96
125	250	8.99	$7.43 \cdot 10^{-6}$	1.74
208	416	15.64	$2.47 \cdot 10^{-7}$	2.78

linear

			ø-time[s]			
H	N	max. error	detailed	reduced	reconstr.	offline-time[s]
16,384	9	$8.92 \cdot 10^{-4}$	2.9	$1.02 \cdot 10^{-5}$	0.259	27.82
262,144	11	$2.15 \cdot 10^{-4}$	621.62	$9.33 \cdot 10^{-4}$	5.679	6,793.21
32,768	9	$3.61 \cdot 10^{-5}$	13.75	$8.32 \cdot 10^{-4}$	1.025	113.85

Publications

- [1] M. Drohmann *Reduced basis model reduction for nonlinear evolution equations* Institute for Computational and Applied Mathematics, Münster, July 2012 (Dissertation)
- [2] M. Drohmann, B. Haasdonk and M. Ohlberger. *Reduced Basis Approximation for Nonlinear Parametrized Evolution Equations based on Empirical Operator Interpolation* SIAM J. Sci. Comput. Society for Industrial and Applied Mathematics, pp. A937-A969 (34), **2012**

http://www.morepas.org/software/

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